

COMLEAM-Software: Modelling Leaching and Environmental Exposure

Michael Burkhardt*, Mirko Rohr, Silvan Gehrig,
Farhad Mehta, Florian Hochstrasser, Olaf Tietje

HSR University of Applied Sciences Rapperswil,
*Institute of Environmental and Process Engineering (UMTEC),
8640 Rapperswil, Switzerland

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Emerging Substances in Building Materials

■ Organic substances in building materials, e.g.

- Biocides (e.g. Terbutryn, Carbendazim, Propiconazol)
- Anti-Root penetration agents (e.g. Mecoprop, MCPA)
- Flame retardants (e.g. TBEP, TCPP, HBCD)
- Plasticisers (e.g. DIDP, DEHP)
- ...

■ Weather conditions relevant for leaching

- Rainfall (400 to 1500 mm)
- Dew (Condensation)
- Temperature (from -20 to +70°C)
- UV-Radiation (degradation)

 **Moisture is the driving force**



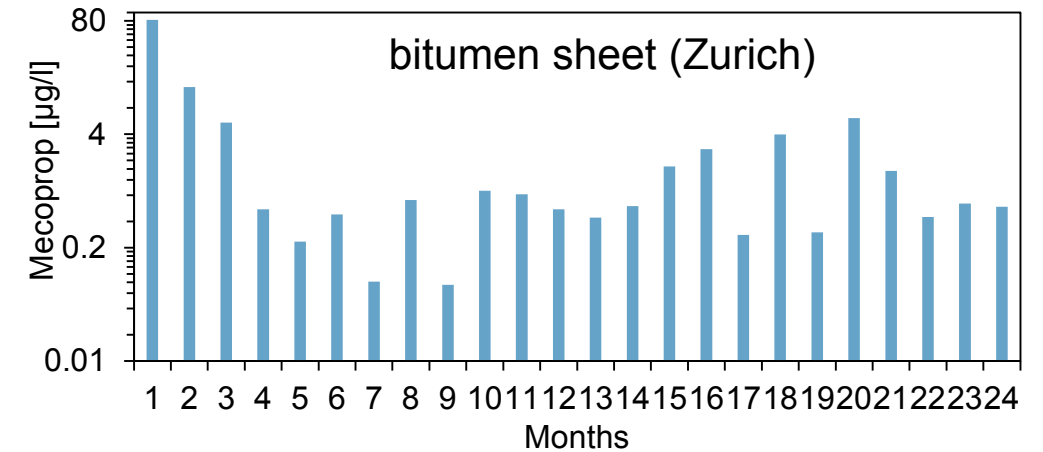
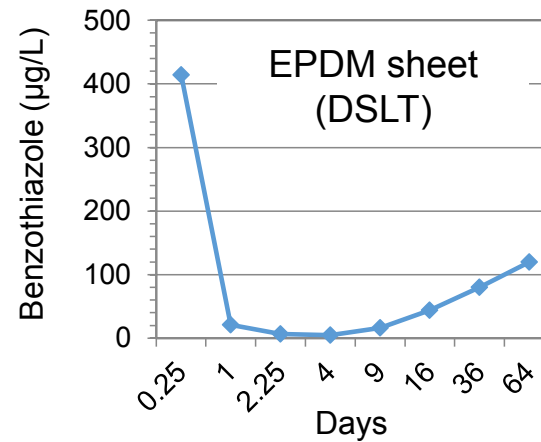
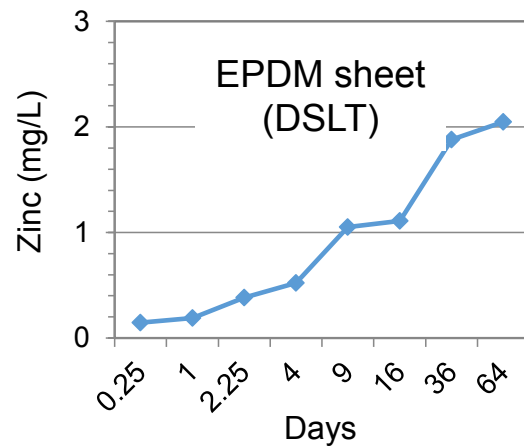
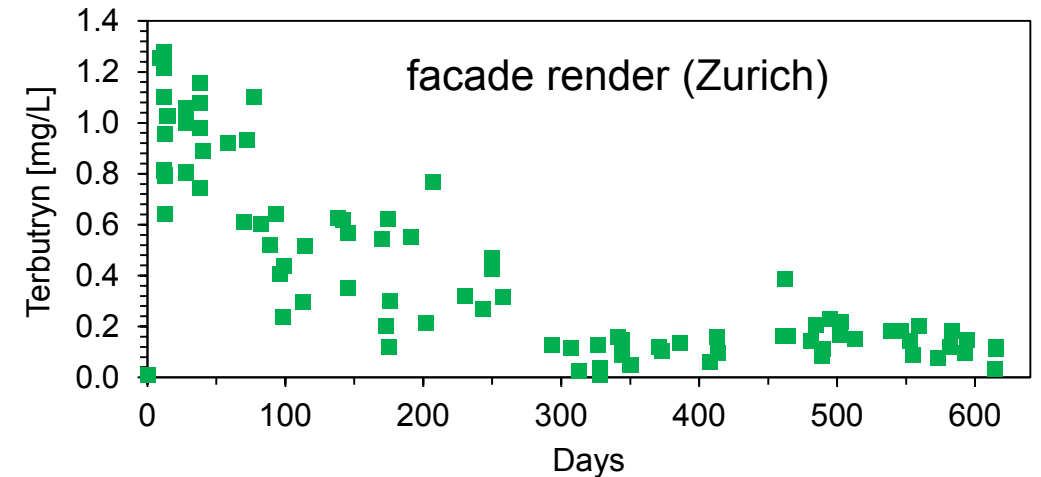
Leaching Studies on Field and Laboratory Scale

Field studies reflecting variability

- Different sizes of panels or buildings
- Different sites and sampling strategies

Laboratory tests according to standards

- DSLT CEN/TS 16637-2 (solid products)
- Immersion test EN16105 (coatings)



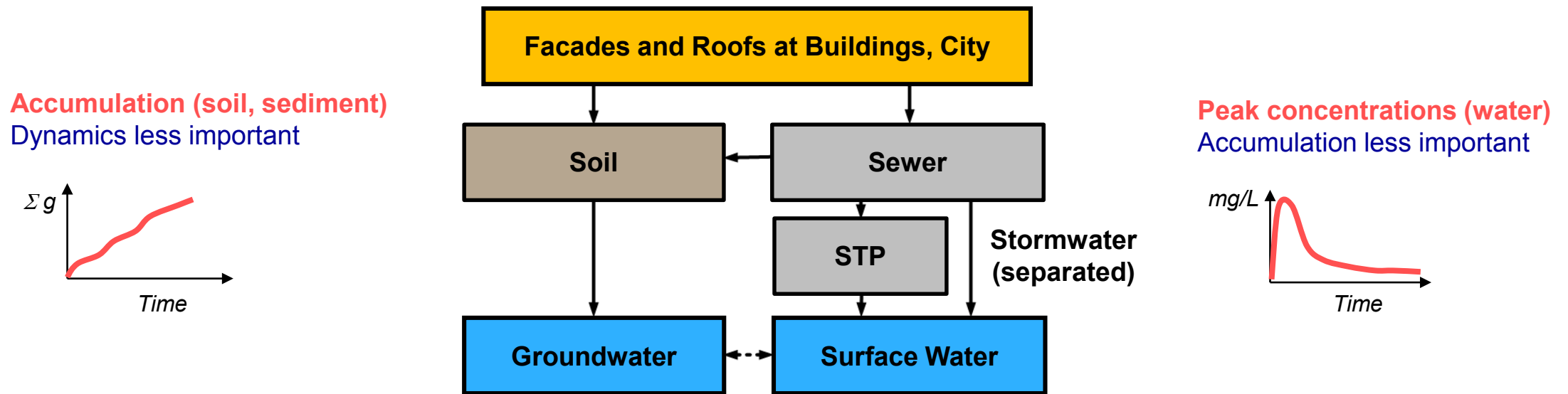
Pathways from Buildings to the Environment

■ Sewer systems are pathways for emissions

- Combined sewer (sewer treatment plant, STP): Treatment of wastewater and stormwater
- Separated sewer: Infiltration to soil or discharge of separated stormwater to surface water

■ Relevance of sewer systems

- In Germany, separated sewers >80 % in North-East and <20 % in South-West
- In Switzerland, about 30 % separated sewers

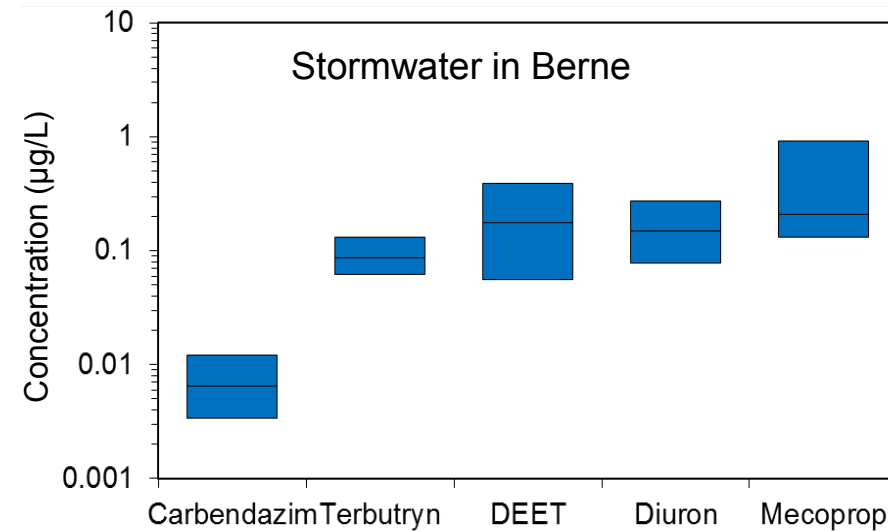
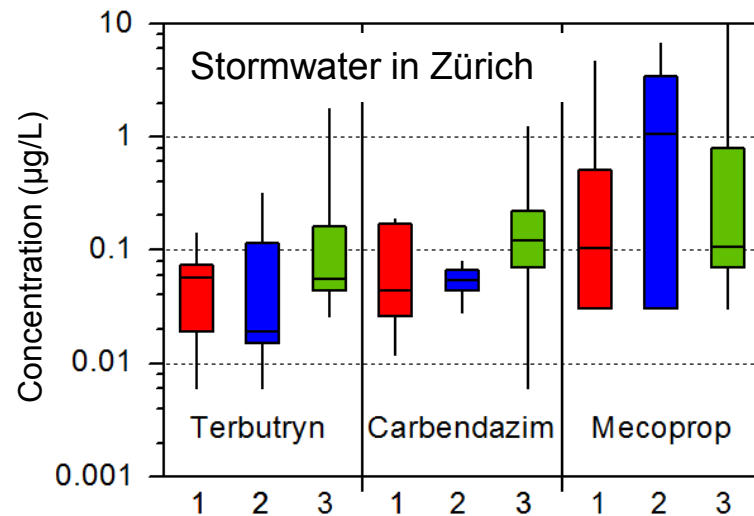


Emissions of Building Materials: Organic Substances in Urban Stormwater

■ Stormwater in urban catchments

- Zürich (20 events) and Berne (25 events) with comparable concentration pattern and following substance order: Mecoprop, Terbutryn, Diuron, Carbendazim
- Lower Emissions at lower temperatures (December – April) and vice versa (May - November)

■ Occurrence related to building structure, construction materials and weather conditions



Burkhardt, M. et al. (2011): Leaching of additives from construction materials to urban storm water runoff. *Water Science & Technology*, 63(9), 1974-1982.

Burkhardt, M. et al. (2017): Behandlung von Regenwasser - Grosstechnische Erfahrung mit unterirdischer Retention und nachgeschaltetem Adsorberfilter. *Aqua und Gas*, 4:78-85.

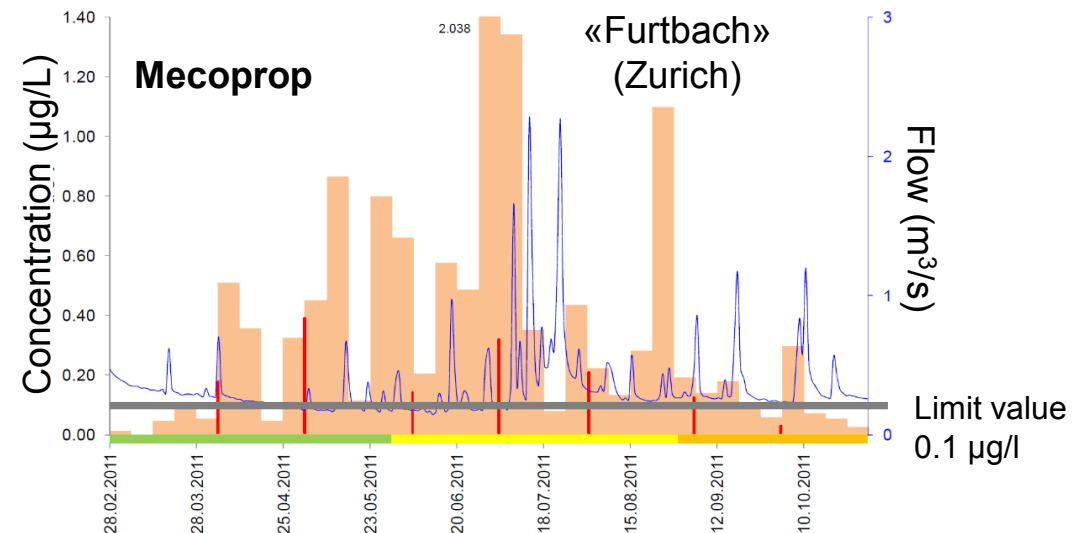
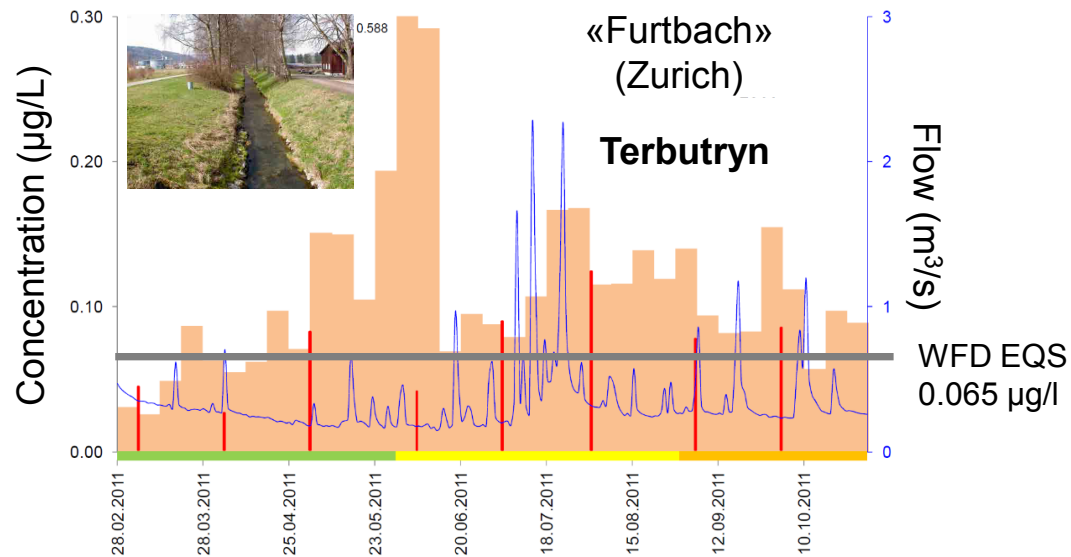
Emissions of Building Materials: Organic Substances in Surface Water

■ Peak pollution by stormwater discharge

- Substances may enter surface water, groundwater and soil

■ Relevant for aquatic organisms and water quality (limit values)

- Terbutryn: At dry and wet weather flow without seasonal pattern (coatings)
- Mecoprop: During wet weather flow without seasonal pattern (bitumen sheets)



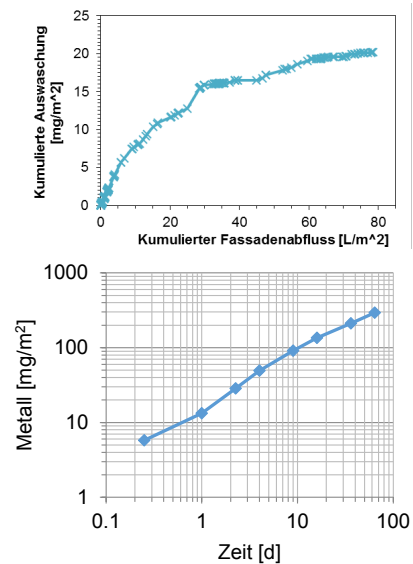
Sinniger et al. (2012): Pestiziduntersuchung, AWEL, Zürich.

How to get an Risk Assessment reflecting the Real World?

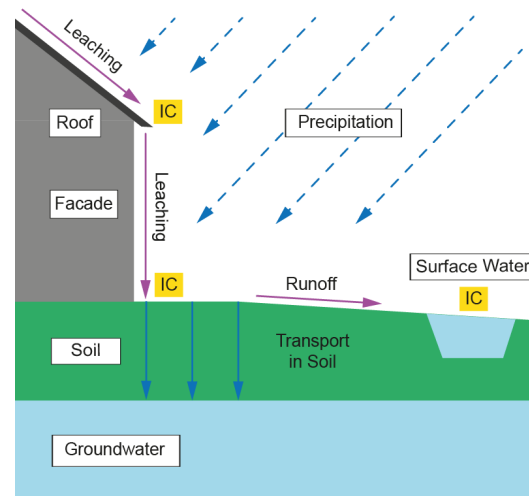
■ Environmental impact of emissions from buildings (CPR, BPR, REAC)

- Time-limited emissions can be measured or predicted: Data available
- Modelling concept and software for upscaling: COMLEAM available
- Boundary conditions representative for European sites: Scenarios needed

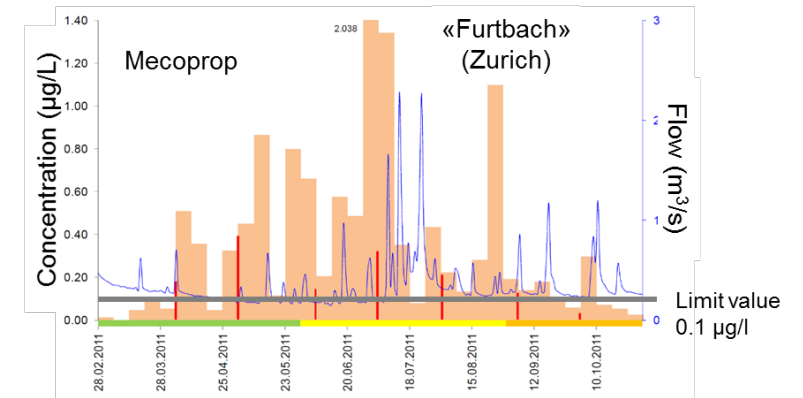
Emission (lab, field)



Software COMLEAM (transfer functions)



Environmental Impact (surface water, groundwater)



Introduction: COMLEAM Software

The screenshot displays the COMLEAM software interface, titled "COMLEAM - CONstruction Material LEACHing Model". The interface is organized into several sections:

- Calculations:** Lists two completed tasks: "ESD City Scenario for PT9 roof membranes calculation for Finished successfully" and "Terbutryn simulation with Hamburg_Fuhsbuettel_20yrs.d Finished successfully". Includes "Show All (2)" and "Add" buttons.
- Reports:** Lists two completed reports: "ESD City Scenario for PT9 roof membranes calculation for substance Carbendazim Finished successfully" and "Terbutryn simulation with Hamburg_Fuhsbuettel_20yrs.dwdDat at Country_OECD_building.cev Finished successfully". Includes "Show All (2)" button.
- Geometries:** A section with a "Show All (2)" and "Add" button.
- Weather Data:** A section with a "Show All (2)" and "Add" button.
- Materials:** Lists two materials: "A facade system with render and paint. Render matle" and "Roof paint, 500 ppm active substance Uncovered roof". Includes "Show All (2)" and "Add" buttons.
- Emission Functions:** Lists three functions: "Log emission function for free terbutryn, r Log", "Log emission function for free diuron, renc Log", and "Log emission function for free terbutryn, r Log". Includes "Show All (5)" and "Add" buttons.
- Notifications:** An empty section on the right side.

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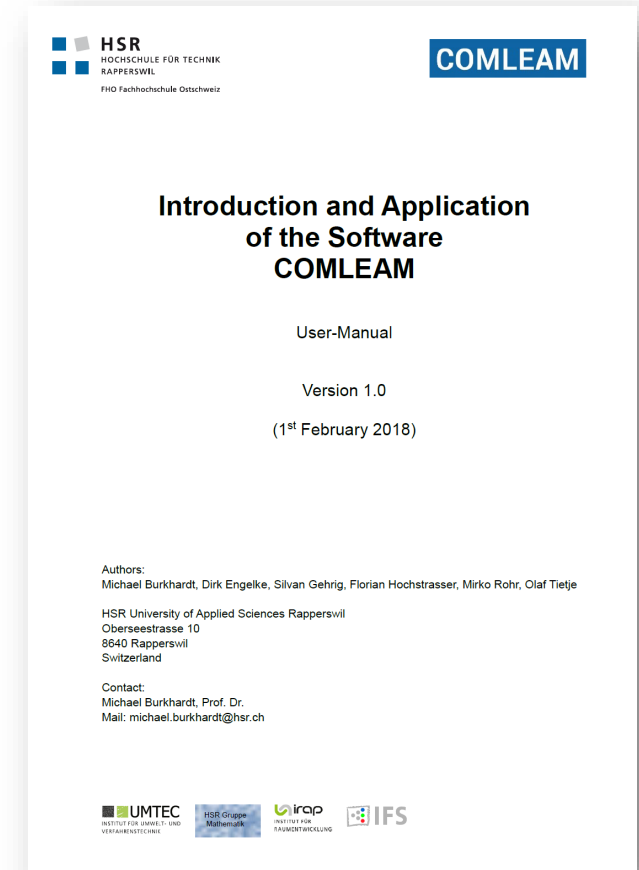
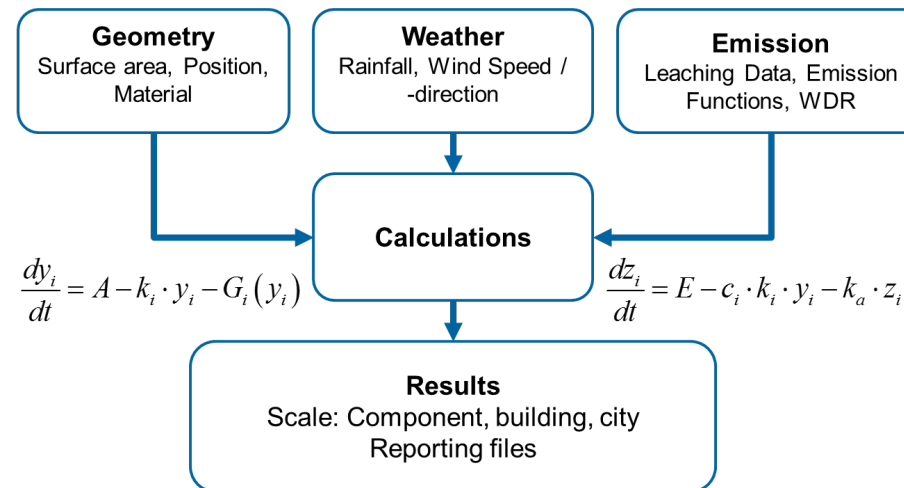
COMLEAM Software: A Modelling Platform

■ Construction Materials Leaching Model (COMLEAM)

- Modelling of leaching of substances to the environment
- Conditions of users interest or predefined scenarios representative for Europe
- Interface is user-friendly
- Manual drafted (V 1.0)

■ Model structure

- Module “Geometry”
 - “Building Material”
- Module “Weather”
- Module “Emission”



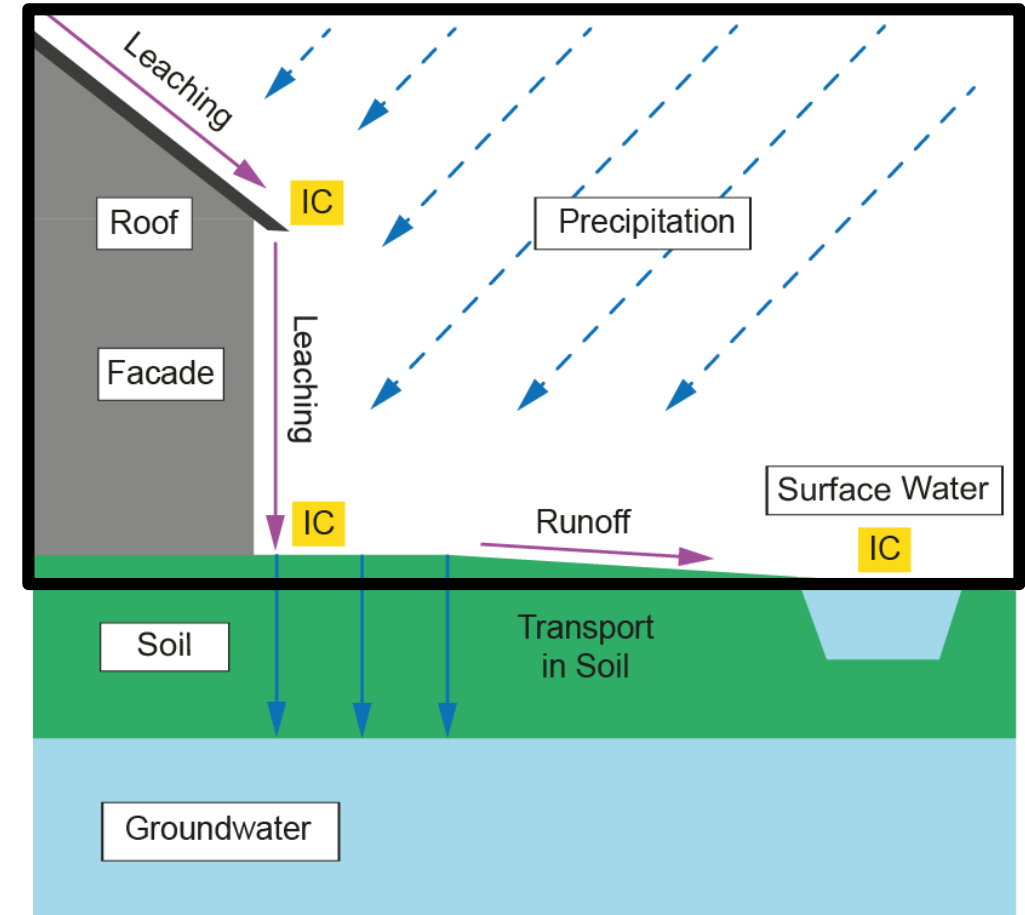
COMLEAM Software: Modelling Leaching and Environmental Exposure

■ System Boundaries

- Leaching of substances (biocides, flame retardants etc.) from construction materials, buildings and cities (roof, façade, etc.)
- Occurrence in surface waters
- Point-of-interest are “interface compartments” (IC)

■ Calculation Methods

- Dynamic Simulation: Temporal resolution of substance release and occurrence (hourly resolution)
 - Details are following in the presentation
- Emission Scenario Documents ESD: Constant emission rates (T1, T2) without local weather conditions
 - Country (single house) for PT 8 and 10
 - City scenario for PT 7, 8, 9 and 10



COMLEAM Software: Module “Geometry”

■ Geometry file

- Components at buildings (1 ... n), e.g. BPR-house, apartment, city
 - Component represent horizontal (e.g. roof, pavement) or vertical surface (e.g. façade, wall)
- Size and Orientation: Height, length, area, exposition (°)
- Optional georeferencing (coordinates)
- Linked to “building materials”

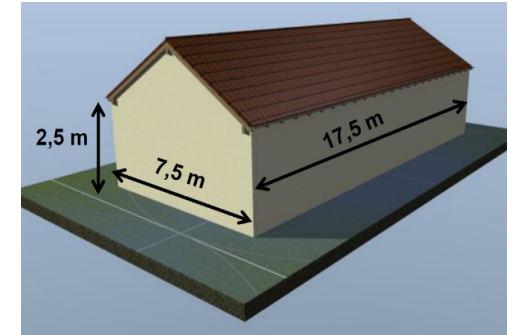
■ Relevance for leaching

- Released amount from surfaces containing substance
 - Substance-free surface areas result in dilution
- Façade orientation is affecting runoff amount and building height the wall factor (WDR)

Component



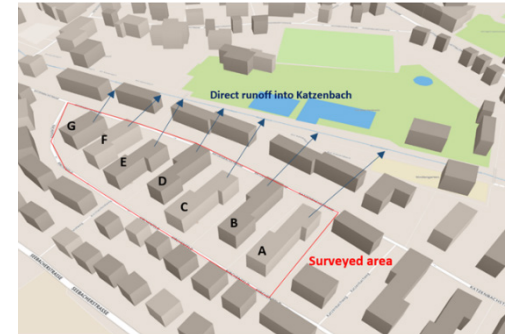
BPR-House



Apartment



City



■ Building material

- Material: Render, paint, polymer membrane etc.
 - Default materials defined for vertical and horizontal surfaces
 - Material combinations possible, e.g. glass and render
- Substance: Terbutryn, Diuron, DCOIT, Zinc, etc.
 - Default substances defined or define your own
 - Combined substances possible, e.g. three different biocides
- Initial concentration: substance amount applied (mg/m²)
- Runoff coefficient ψ : Water losses by splashing, absorption, evaporation
 - Runoff coefficient is defined per material subtype

■ Relevance for exposure

- Emission function is based on a certain substance
- Environmental risk is related to leaching behavior and amount of substance



| Biocide | Solubility (mg/L) | logPow | Persistence |
|------------------|-------------------|--------|-------------|
| Terbutryn | 22 | 3.7 | high |
| Diuron | 35 | 2.7 | high |
| Isoproturon | 70 | 2.5 | high |
| DCOIT | 14 | 4.9 | medium |
| OIT | 480 | 2.4 | low |
| IPBC | 168 | 2.4 | low |
| Carbendazime | 8 | 1.6 | medium |
| Zinc pyriithione | 8 | 0.9 | medium |

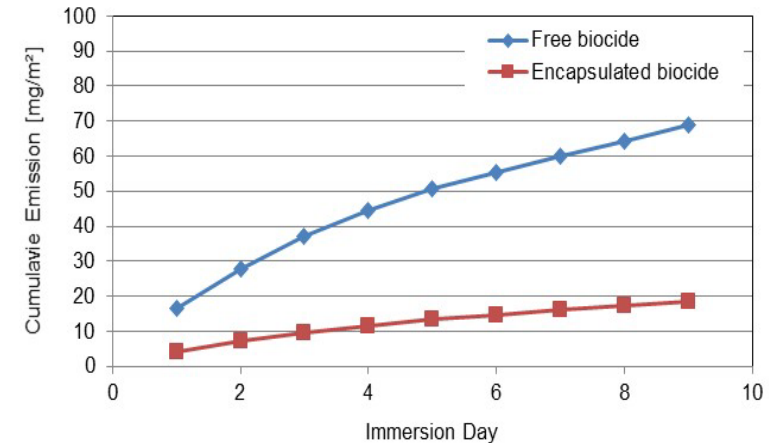
■ Transfer of leaching data

- Leaching data: measured cumulated runoff [L/m^2] and cumulated emission [mg/m^2]
- Emission function needed for upscaling leaching
 - Defaults are log, double loglinear, diffusion-controlled, limited growth, and linear or set your own
 - Log function gives best fit (Tietje et al, 2018)
- Parameterization of leaching data
 - Parameters derived by non-linear regression (nls)

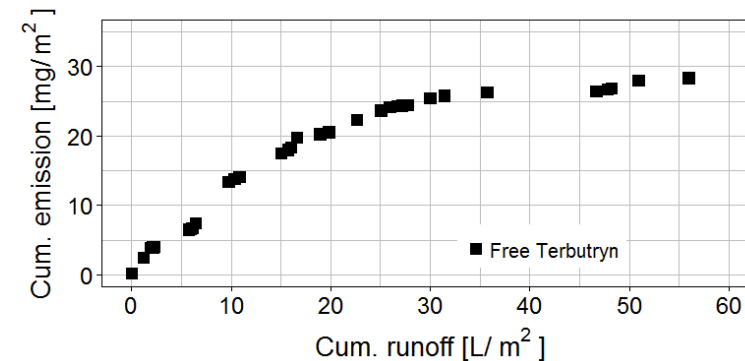
■ Relevance for exposure assessment

- Parameters are used for up-scaling the emission
 - Buildings (test panel, building, city etc.)
 - Prediction for long-term or different sites

Lab Data (EN16105, DSLT)



Field Data



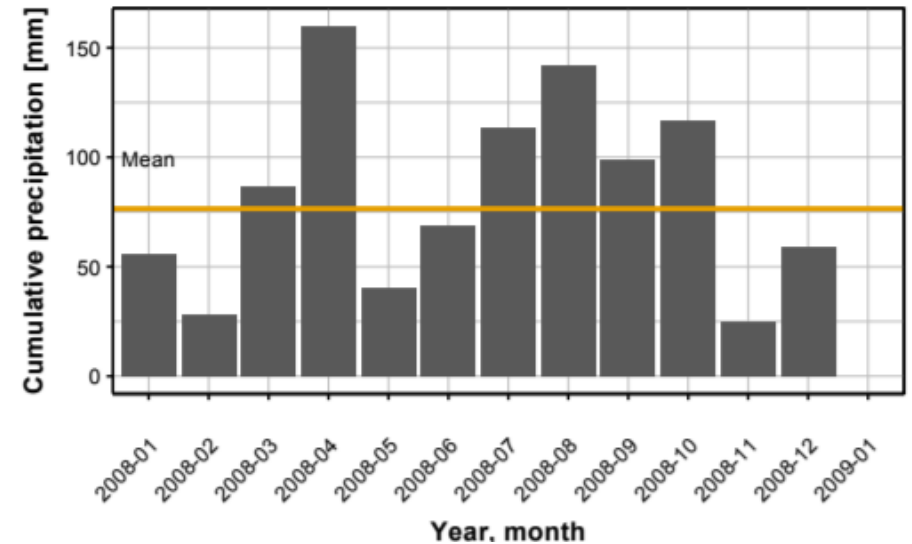
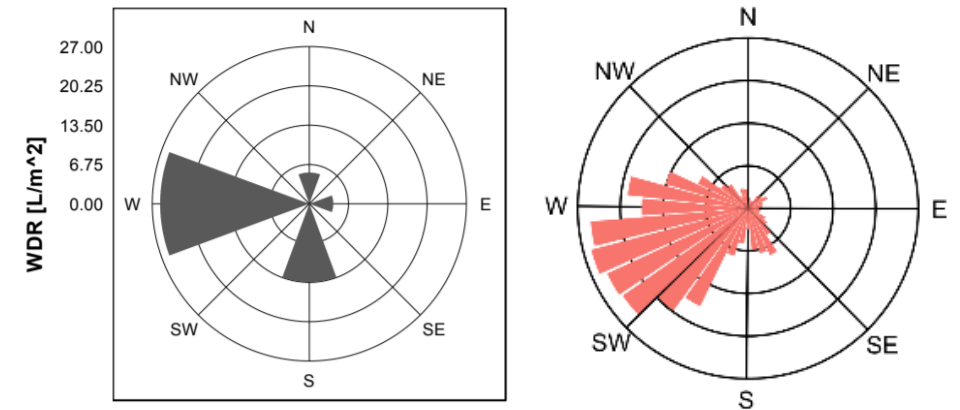
COMLEAM Software: Module “Weather” and Surface Water Compartment

■ Weather data

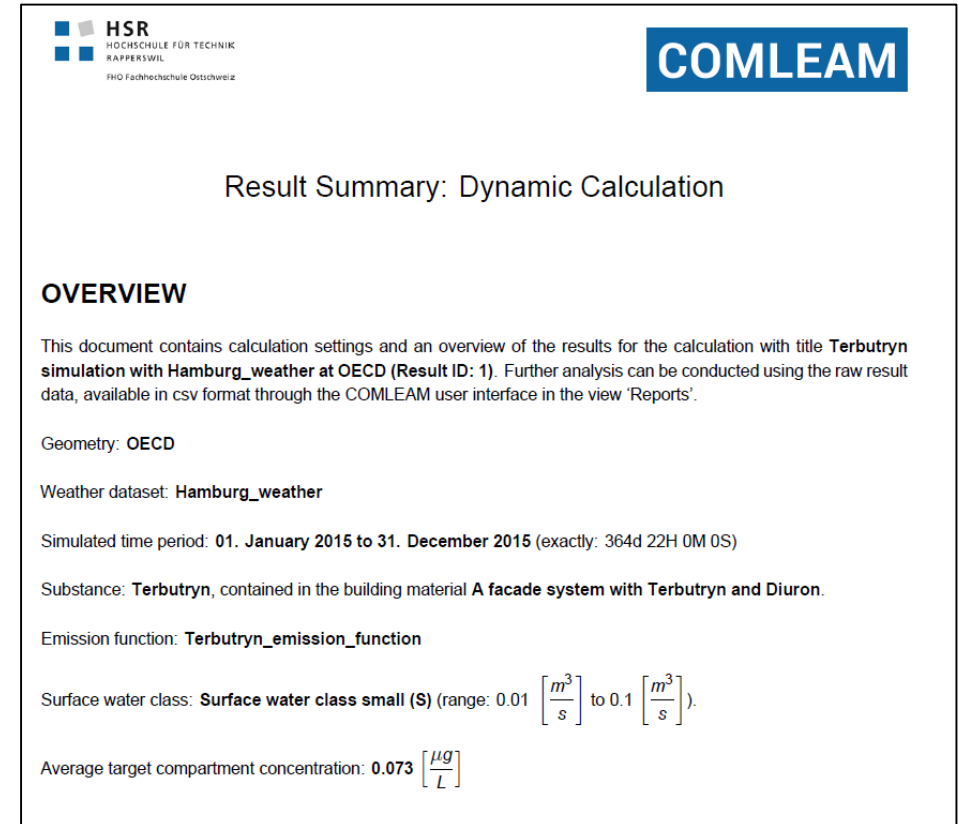
- Data files of commercial stations or own data
- Wind driven rain (WDR, ISO 15927-3:2009) calculation depends on wind direction and wind speed
 - Exposure (E, W, N, S)
 - Height of Building
 - Position to other buildings and location

■ Receiving surface water

- Default classes are provided
 - Class S: $< 0.1 \text{ m}^3/\text{s}$ ($< 8.6 \text{ m}^3/\text{d}$)
 - Class M: $0.1 - 1 \text{ m}^3/\text{s}$
 - Class L: $> 1 \text{ m}^3/\text{s}$ ($> 86 \text{ m}^3/\text{d}$)



- **Reporting document (13 pages)**
 - Summary of all simulation settings and results
 - Standardized PDF-document
 - Get the report by “*Download Report*”
- **Output data**
 - Containing all information of the simulation
 - Useful for individual data processing
 - Import file for other compartment models (e.g. PELMO, PEARL)
 - Get the data as .csv-files by “*Download Data*”



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COMLEAM

Result Summary: Dynamic Calculation

OVERVIEW

This document contains calculation settings and an overview of the results for the calculation with title **Terbutryn simulation with Hamburg_weather at OECD (Result ID: 1)**. Further analysis can be conducted using the raw result data, available in csv format through the COMLEAM user interface in the view 'Reports'.

Geometry: OECD

Weather dataset: **Hamburg_weather**

Simulated time period: **01. January 2015 to 31. December 2015** (exactly: 364d 22H 0M 0S)

Substance: **Terbutryn**, contained in the building material **A facade system with Terbutryn and Diuron**.

Emission function: **Terbutryn_emission_function**

Surface water class: **Surface water class small (S)** (range: $0.01 \left[\frac{m^3}{s} \right]$ to $0.1 \left[\frac{m^3}{s} \right]$).

Average target compartment concentration: **0.073** $\left[\frac{\mu g}{L} \right]$

Conclusion: COMLEAM Software

- **Dynamic simulation of time-limited leaching from construction materials, buildings and cities using lab/field data and occurrence of substances in surface waters**
 - Multiple runs reflecting real application conditions and environmental risk over life-time (e.g. 20 years)
- **Initial scenarios are prepared and tested – EU scenarios can be prepared with support of partners**
 - Default values set and benchmark data provided for refinements (beneficial for product classification !)
- **Web-based Version will be online available in September 2019**
 - New Version 2.0 (new tools integrated)
- **Open platform for “creative” simulations of scientists or evaluation of reduction measures**
 - Coupling to 3D-GIS, soil models or hydrological models of sewer networks
- **Users of COMLEAM from authorities, industry and sciences are supported for free of charge**
 - Technical support is guaranteed

A scenic view of a town with a large church and snow-capped mountains in the background, reflected in a lake. The town is situated on the shore of a calm body of water, and the mountains are covered in snow. The church has a prominent tower and is a central feature of the town's skyline. The water is still, creating a clear reflection of the buildings and the mountains. The sky is a clear, light blue, suggesting a bright day.

Thank you for your attention!

E- Mail: michael.burkhardt@hsr.ch